



# The weighted Kendall and high-order kernels for permutations

Yunlong Jiao  
University of Oxford

Jean-Philippe Vert  
MINES ParisTech

ICML @ Stockholm, 11 July 2018

## Ranking data is everywhere

- ▶ Rank data, e.g., preference survey:



- ▶ Ranking extracted from data, e.g., gene expression:

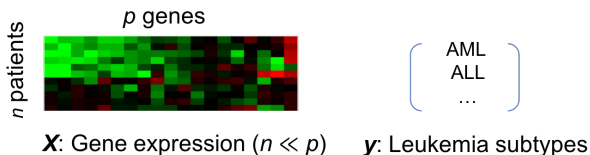
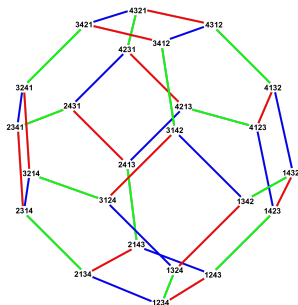


Figure: “If the expression of two genes  $SPTAN1 \geq CD33$ , then ALL; otherwise AML” gives accuracy of 93.80% [Tan et al., 2005].

# Mathematical difficulty



- ▶ A (total) ranking is a permutation

$$\sigma : [1, n] \rightarrow [1, n]$$

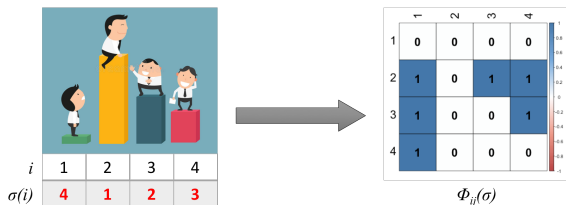
such that  $\sigma(i) = \text{rank of item } i$ .

- ▶  $\mathbb{S}_n$  the symmetric group with composition

$$(\sigma_1\sigma_2)(i) = \sigma_1(\sigma_2(i))$$

with cardinality  $|\mathbb{S}_n| = n!$ .

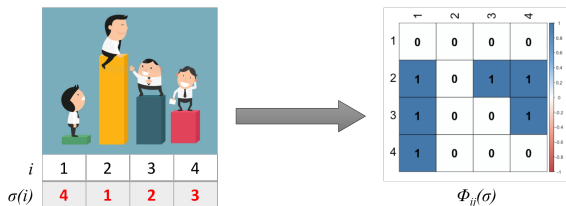
# The Kendall embedding



- The **Kendall embedding** is an  $n^2$ -dimensional **Euclidean** embedding:

$$\Phi_{\tau} : \mathbb{S}_n \rightarrow \mathbb{R}^{n \times n}; \quad (\Phi_{\tau}(\sigma))_{i,j} = \begin{cases} 1 & \text{if } \sigma(i) < \sigma(j), \\ 0 & \text{otherwise.} \end{cases}$$

# The Kendall embedding



- Quantities using Kendall embedding [Jiao and Vert, 2015]:

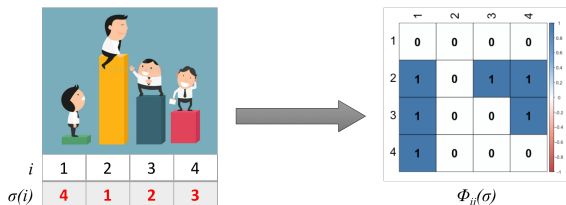
Kendall's  $\tau$  correlation:  $K_\tau(\sigma, \sigma') \propto \langle \Phi_\tau(\sigma), \Phi_\tau(\sigma') \rangle$

Kendall's  $\tau$  distance:  $d_\tau(\sigma, \sigma') \propto \|\Phi_\tau(\sigma) - \Phi_\tau(\sigma')\|^2$

Mallows distribution:  $\mathbb{P}(\sigma) \propto \exp\{-\lambda \|\Phi_\tau(\sigma) - \Phi_\tau(\pi)\|^2\}$   
for mode  $\pi \in \mathbb{S}_n$  and dispersion  $\lambda > 0$

(Nonlinear) predictive model:  $h(\sigma) = \langle B, \Phi_\tau(\sigma) \rangle$   
for coefficients  $B \in \mathbb{R}^{n \times n}$

# The Kendall kernel



- Quantities using Kendall embedding [Jiao and Vert, 2015]:

**Kendall kernel:**

$$K_{\tau}(\sigma, \sigma') \propto \langle \Phi_{\tau}(\sigma), \Phi_{\tau}(\sigma') \rangle$$

Kendall's  $\tau$  distance:

$$d_{\tau}(\sigma, \sigma') \propto \|\Phi_{\tau}(\sigma) - \Phi_{\tau}(\sigma')\|^2$$

Mallows distribution:

$$\mathbb{P}(\sigma) \propto \exp \left\{ -\lambda \|\Phi_{\tau}(\sigma) - \Phi_{\tau}(\pi)\|^2 \right\}$$

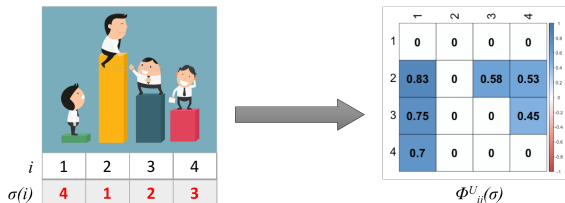
for mode  $\pi \in \mathbb{S}_n$  and dispersion  $\lambda > 0$

**Kernel machine** (Classification, regression, clustering, etc.):

$$h(\sigma) = \sum_{i=1}^N \alpha_i K_{\tau}(\sigma, \sigma_i)$$

for coefficients  $\alpha \in \mathbb{R}^N$  (“kernel trick”)

# The weighted Kendall embedding



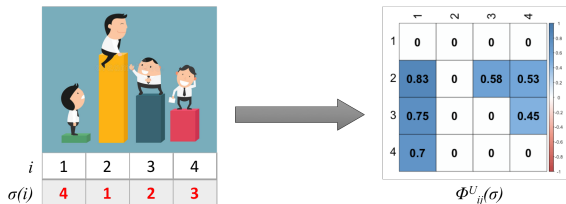
- The **weighted Kendall embedding** is:

$$\Phi^U : \mathbb{S}_n \rightarrow \mathbb{R}^{n \times n}; \quad \left( \Phi^U(\sigma) \right)_{i,j} = \begin{cases} U_{\sigma(i), \sigma(j)} & \text{if } \sigma(i) < \sigma(j), \\ 0 & \text{otherwise,} \end{cases}$$

where  $U \in \mathbb{R}^{n \times n}$  is a **weight matrix** such as

- Top- $k$   $U_{i,j} = 1$  iff  $i, j \leq k$ , for rank threshold  $k$ .
- Additive  $U_{i,j} = u_i + u_j$ , for rank discounts  $u \in \mathbb{R}^n$ .
- Multiplicative  $U_{i,j} = u_i u_j$ , for rank discounts  $u \in \mathbb{R}^n$ .

# The weighted Kendall kernel



- The **weighted Kendall kernel**:

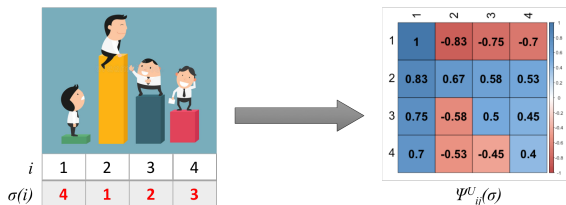
$$K_U(\sigma, \sigma') \propto \langle \Phi^U(\sigma), \Phi^U(\sigma') \rangle$$

is a weighted Kendall's  $\tau$  correlation, which is:

- ✓ Symmetric.
- ✓ Invariant to shuffling of the index  $i$ .
- ✓ **Fast to compute** in  $O(n \log n)$  time.
- ✓ **Positive definite**, enabling to use **all** kernel machines (classification, regression, clustering, etc.)



# Learning the weights



- ▶ In general, the weighted embedding and kernel are:

$$\Phi^U : \mathbb{S}_n \rightarrow \mathbb{R}^{n \times n}; \quad \left( \Phi^U(\sigma) \right)_{i,j} = U_{\sigma(i), \sigma(j)},$$

$$G_U(\sigma, \sigma') \propto \left\langle \Phi^U(\sigma), \Phi^U(\sigma') \right\rangle.$$

- ▶ The weight matrix  $U \in \mathbb{R}^{n \times n}$  can be **learned jointly** with the coefficients of a kernel machine, by solving a **non-convex** optimization via:
  - Alternative optimization between weights and coefficients.
  - Low-rank approximation [Le Morvan and Vert, 2017].

## Going beyond item pairs

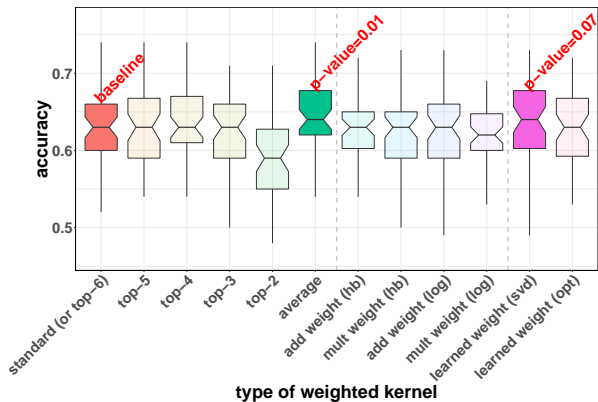
- ▶ The **order-3** (or higher) weighted embedding and kernel are:

$$\Phi^{\mathcal{U}} : \mathbb{S}_n \rightarrow \mathbb{R}^{n \times n \times n}; \quad (\Phi^{\mathcal{U}}(\sigma))_{i,j,k} = \mathcal{U}_{\sigma(i),\sigma(j),\sigma(k)},$$
$$G_{\mathcal{U}}(\sigma, \sigma') \propto \langle \Phi^{\mathcal{U}}(\sigma), \Phi^{\mathcal{U}}(\sigma') \rangle .$$

- ▶ The **weight tensor**  $\mathcal{U} \in \mathbb{R}^{n \times n \times n}$  can also be **learned** in a data-driven way, similarly to the order-2 case.

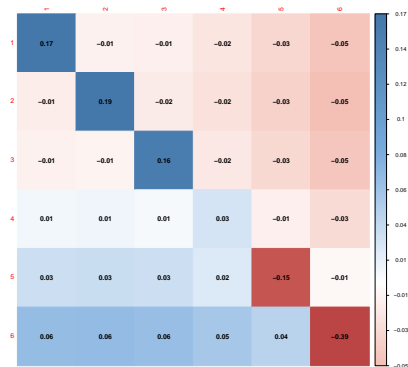
## Real-data experiments: Prediction accuracy

- ▶ Eurobarometer survey data [Christensen, 2010]:
  - >12k participants ranked the importance of 6 sources of information
  - Binary classification problem: predict age group (>40yo vs <40yo) from ranking



## Real-data experiments: Weights learned

- ▶ Eurobarometer survey data [Christensen, 2010]:
  - >12k participants ranked the importance of 6 sources of information
  - Binary classification problem: predict age group (>40yo vs <40yo) from ranking



# Conclusion

- ▶ We have studied
  - ✓ Euclidean embeddings and positive definite kernels for permutations, which are
    - ✓ weighted and high-order extensions to Kendall's  $\tau$  correlation, where
      - ✓ weights can be learned systematically in a data-driven way.



# References I



Pictures are downloaded from internet (no copyright infringement is intended).  
<https://www.dreamstime.com/stock-illustration-chart-showing-rank-people-lives-most-successful-one-top-here-illustration-image53416790>;  
<https://www.dreamstime.com/stock-photos-speed-limit-35-image754943>.



Christensen, T. (2010).  
Eurobarometer 55.2: Science and technology, agriculture, the euro, and internet access, may-june 2001.  
<https://doi.org/10.3886/ICPSR03341.v3>.



Jiao, Y. and Vert, J.-P. (2015).  
The Kendall and Mallows kernels for permutations.  
In *Proceedings of the 32nd International Conference on Machine Learning (ICML)*, volume 37 of *Proceedings of Machine Learning Research (PMLR)*, pages 1935–1944.



Le Morvan, M. and Vert, J.-P. (2017).  
Supervised quantile normalisation.  
*arXiv preprint arXiv:1706.00244*.



Tan, A. C., Naiman, D. Q., Xu, L., Winslow, R. L., and Geman, D. (2005).  
Simple decision rules for classifying human cancers from gene expression profiles.  
*Bioinformatics*, 21(20):3896–3904.